

Delone Sets: Local Identity and Global Symmetry ^{*}

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To Friends who love and do Geometry

Abstract

In the paper we present a proof of the local criterion for crystalline structures which generalizes the local criterion for regular systems. A Delone set is called a crystal if it is invariant with respect to a crystallographic group. So-called locally antipodal Delone sets, i.e. such sets in which all $2R$ -clusters are centrally symmetrical, are considered. It turns out that the local antipodal sets have crystalline structure. Moreover, if in a locally antipodal set all $2R$ -clusters are the same the set is a regular system, i.e. a Delone set whose symmetry group operates transitively on the set.

1 Introduction

This paper continues an investigative line started in the pioneering work [5] on local conditions in a Delone set X to imply that set X is either a regular system, i.e. a crystallographic orbit of a single point, or a crystal, i.e. the orbit of a few points. On Fig. 1 one can see the set X_1 of blue points which sit at nodes of the square grid and the set X_2 of red point quadruples. Each of these sets is a regular system because each of them is an orbit of a 2D-crystallographic group $p4m$ (the full group of the standard square grid on the plane). The union $X = X_1 \cup X_2$ of the sets X_1 and X_2 is a crystallographic orbit of two points, i.e. it is an example of a crystal.

So, a mathematical model of an ideal crystal uses two concepts: the concept of the Delone set (which is of local character) and the concept of the crystallographic group (which is of global character). After Fedorov [8] a mathematical model of a mono-crystalline matter is defined as a Delone set which is invariant with respect to some crystallographic group. One should emphasize that under this definition the well-known periodicity of crystal in all 3 dimensions is not an additional requirement. By the famous Schönflies-Bieberbach theorem [3,4], any space group contains a translational subgroup with a finite index.

Since the crystallization is such a process that results from mutual interaction of nearby atoms, it is believed (R. Feynman, N.V. Belov, et al) that the long-range

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order of atomic structures of crystals (and quasi-crystals too) comes out of local rules restricting the arrangement of nearby atoms. R. Feynman wrote ([10], Ch. 30): "when the atoms of matter are not moving around very much, they get stuck together and arrange themselves in a configuration with as low an energy as possible. If the atoms in a certain place have found a pattern which seems to be of low energy, then the atoms somewhere else will probably make the same arrangement. For these reasons, we have in a solid material a repetitive pattern of atoms. In other words, the conditions in a crystal are this way: The environment of a particular atom in a crystal has a certain arrangement, and if you look at the same kind of an atom at another place farther along, you will find one whose surroundings are exactly the same. If you pick an atom farther along by the same distance, you will find the conditions exactly the same once more. The pattern is repeated over and over again, and, of course, in three dimensions." The crystallographer N.V. Belov also suggested similar arguments in a problem "on the 501st element".

However, before 1970's there were no whatever rigorous results to explain a link between properties of local patterns and the global order in the internal structure of crystals until Delone and his students initiated developing the local theory of crystals [5]. One of two main aims of the local theory was (and is) rigorous derivation of space group symmetry of a crystalline structure from the pairwise identity of local arrangements around each atom.

One should mention that the link between the identity of local fragments of a structure and global order of the structure seemed obvious, and searching for an exact wording of this connection and its rigorous proof were

seen a purely abstract goal that would be of interest only to mathematicians.

However, the subsequent discovery of non-periodic Penrose patterns (1977) and the discovery by D. Shechtman of real quasicrystals (1982, Nobel Prize in 2011) have showed that there are non-periodic structures which are as locally identical as crystals. These discoveries suggest that the connection between the local identity and the global order is not so obvious. One of the goals of the local theory of global order was to look for right wordings of statements and then prove them.

The local theory has been developed for Delone sets as well as for polyhedral tilings, including combinatorial aspects of the theory (see e.g. [11,12,13]).

The paper is organized as follows. In the next section we give definitions of all necessary concepts and short survey of some earlier results. Then we give formulation of the local criterion for a crystal and of several new "local" theorems on locally antipodal Delone sets (Theorems 1– 5), which will be proved in concluding sections of the paper.

2 Basic Definitions and Results

Definition 2.1. A point set $X \subset \mathbb{R}^d$ is called a *Delone set* with parameters r and R , where r and $R > 0$, (or an (r, R) -system, see [1,2]), if two conditions hold:

(1) an open d -ball $B_y^o(r)$ of radius r centered at an *arbitrary* point $y \in \mathbb{R}^d$ contains at most one point from X :

$$|B_y^o(r) \cap X| \leq 1; \tag{r}$$

(2) a closed d -ball $B_y(R)$ of radius R centered at an arbitrary point y contains at least one point from X :

$$|B_y(R) \cap X| \geq 1. \quad (R)$$

We note that by condition (r) the distance between any two points x and $x' \in X$ is not less than $2r$.

For $x \in X$ we denote $C_x(\rho) := X \cap B_x(\rho)$ and will call the set $C_x(\rho) \subset X$ a ρ -cluster of point x . Thus, a ρ -cluster $C_x(\rho)$ consists of all points of X that are placed from x at distance at most ρ . It is easy to see that for $\rho < 2r$ $C_x(\rho) = \{x\}$. It is well-known that for $\rho \geq 2R$, the ρ -cluster $C_x(\rho)$ of any point $x \in X$ has the full rank: the dimension of $\text{conv}(C_x(\rho)) = d$

In principle, the ρ -cluster $C_x(\rho)$ is considered as a pair (the center x , the point set $C_x(\rho)$). However, since notation $C_x(\rho)$ contains information on the center x we can miss the notation of a cluster as the pair. We emphasize that we distinguish between ρ -clusters $C_x(\rho)$ and $C_{x'}(\rho)$ of different points x and x' , even if the two sets generally may coincide (see Fig. 1).

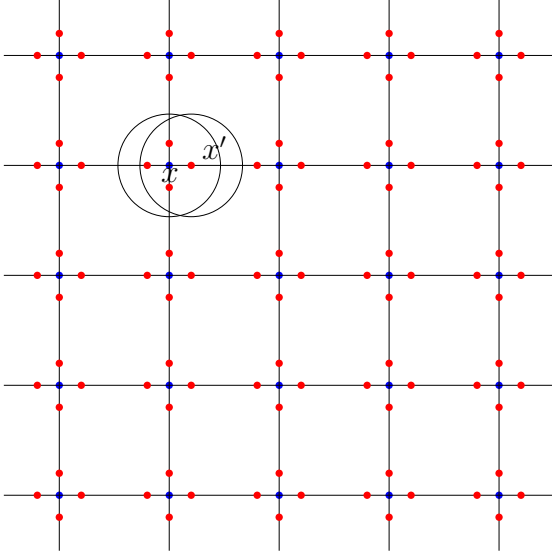


Fig. 1

Definition 2.2. Two ρ -clusters $C_x(\rho)$ and $C_{x'}(\rho)$ are called *equivalent*, if there is an isometry $g \in O(d)$ such that

$$g : x \mapsto x' \text{ and } g : C_x(\rho) \rightarrow C_{x'}(\rho).$$

We emphasize that the requirement of equivalence of two clusters is some stronger than just of congruence of sets of points that enter these clusters. Two clusters depicted on fig.1 around two points x and x' coincide as subsets of X . However, since this subset of X surrounds the points x and x' in different ways it is natural to distinguish between the ρ -clusters $C_x(\rho)$ and $C_{x'}(\rho)$. Indeed, the clusters $C_x(\rho)$ and $C_{x'}(\rho)$ are non-equivalent because there is no isometry that moves both point x and cluster $C_x(\rho)$ into point x' and cluster $C_{x'}(\rho)$, respectively.

In a Delone set for any $\rho > 0$ a set of clusters is partitioned into classes of equivalent ρ -clusters. For any given ρ if $\rho < 2r$, ρ -cluster at any point of X consists of a single

point: $C_x(\rho) = \{x\}$, i.e. all "small" ρ -clusters in X are equivalent. Given Delone set X , we denote by $N(\rho)$ the cardinality of a set of equivalence classes of ρ -clusters in X .

We have in any Delone set X $N(\rho) = 1$ for $\rho < 2r$. However, for larger ρ , $\rho > 2r$, $N(\rho)$ can be generally infinite.

Definition 2.3. A Delone set X is said to be *of finite type* if for each $\rho > 0$ the number $N(\rho)$ of classes of ρ -clusters is finite.

As we said, for any Delone set X function $N(\rho)$ is always defined and equal to 1 for all $\rho < 1$. It is not hard to prove the following:

Statement 2.1. *Function $N(\rho) < \infty$ for all $\rho > 0$ if $N(2R) < \infty$.*

The key reason of this fact is as follows. Given X , the condition $N(2R) < \infty$ implies, that in a Delone tiling for set X (see [2]) there are just finitely many pairwise non-congruent tiles. Next, we note that in the Delone tiling, that is, importantly, face-to-face, any two convex finite d -polyhedra P and Q that share a common $(d-1)$ -face can form just finitely many non-congruent pairs (P, Q) . From here it follows in the Delone tiling with $N(2R) < \infty$ for any ρ there are just finitely many non-congruent fillings of a ball $B_x(\rho)$. The finiteness of different parts of the tiling of size ρ implies the finiteness of $N(\rho)$.

Now we take a point $x \in X$ and the cluster $C_x(2R)$. Points of the cluster uniquely determine all Delone cells for X that meet at point x . Now, since $N(2R) < \infty$ the number of non-congruent Delone cells in a Delone tiling for X is finite. Due to this finiteness and also to above-mentioned finiteness of the number of pairs of P and Q glue along their common hyperface. These two sorts of finiteness imply just finite number of non-congruent fillings of a ball of radius ρ with Delone tiles. It follows that every $2R$ -cluster $C_x(2R)$ admits just a finite number of non-congruent extensions to a ρ -cluster $C_x(\rho)$. Since, by assumption, there are finitely many pairwise non-congruent $2R$ -clusters, then there are finitely many ρ -clusters for any given $\rho > 0$.

From now on, we will consider Delone sets of finite type only. We note that in such a Delone set the number $N(\rho)$ of ρ -clusters is a positive, integer-valued, non-decreasing, piece-wise constant function, continuous on the right.

Very important examples of Delone sets are the so-called *regular systems* and *crystals*. The concept of the regular system was studied by E.S.Fedorov [8]. Regular systems are discrete homogenous sets which looks the same up to infinity from any its point. Here is an equivalent definition in terms of a Delone set.

Definition 2.4 A *regular system* is a Delone set $X \subset \mathbb{R}^d$ whose symmetry group acts transitively, i.e. for any two points x and $x' \in X$ there is an isometry $g \in Iso(d)$ such that

$$g : x \mapsto x' \text{ и } g : X \rightarrow X \quad .$$

Recall that a group $G \subset Iso(d)$ is called a *crystallographic group* if

- (1) G operates discontinuously at each point $y \in \mathbb{R}^d$, i.e. if for any point $y \in \mathbb{R}^d$ orbit $G \cdot y$ is a discrete set;
- (2) G has a compact fundamental domain.

One can reformulate the definition of a regular set in terms of a crystallographic group. We emphasize that in the following statement we do not require that X is a Delone set. This condition results from properties of a crystallographic group.

Statement 2.2. *A set $X \subset \mathbb{R}^d$ is a regular system if and only if the set X is an orbit of a point $x \in \mathbb{R}^d$ with respect to a crystallographic group $G \subset Iso(d)$.*

A regular set is an important particular case of the more general concept of a crystal.

Definition 2.5. A crystal is a Delone set X such that X is a finite collection of orbits with respect to its symmetry group $Sym(X)$: $X = Sym(X) \cdot X_0$, where X_0 is a finite point set.

It is not hard to prove that the symmetry group of a crystal is a crystallographic group. Thus we have the following statement.

Statement 2.3. *A set $X \subset \mathbb{R}^d$ is a crystal if and only if it is an orbit of a finite set X_0 with respect to a crystallographic group G , i.e. $X = G \cdot X_0$.*

These classes of Delone sets can be described via the cluster counting function $N(\rho)$ as follows. A Delone set of finite type is a regular system if and only if $N(\rho) \equiv 1$ on R_+ . A Delone set is a crystal if and only if its cluster counting function is bounded:

$$N(\rho) \leq m < \infty, \quad \text{where } m \leq |X_0|.$$

If $m = 1$, then a crystal is a regular system.

The above-mentioned definitions of a regular system and a crystal go back to Fedorov, [8]. Earlier, before Fedorov's work, a crystal had been considered as a set of pairwise congruent and parallel lattices. The definition of a crystal in terms of regular systems seemed to generalize the Haui-Bravais concept of a crystal as a 3D periodic Delone set.

However, indeed, due to the Schönflis-Bieberbach theorem, the more general structure of a regular system is also the union of lattices. Therefore, due to the Fedorov definition, a crystal is the union of several lattices exactly as in the Haui-Bravais approach.

Indeed, let h be the index of the translational subgroup of a crystallographic group $G \subset Iso(d)$, $|X_0|$ the number of points in X_0 , then a crystal $G \cdot X_0$ splits into m pairwise congruent and parallel lattices of rank d :

$$G \cdot X_0 = \cup_i^m (T \cdot x_i \cup T \cdot g_2(x_i) \cup \dots \cup T \cdot g_h(x_i)), \quad x_i \in X_0.$$

We note that m is strictly smaller than $h \cdot |X_0|$ if some points x_i and x_j in X_0 belong to one G -orbit.

Now we define the group $S_x(\rho)$ of ρ -cluster $C_x(\rho)$ as a subgroup of $Iso(d)$ to consist of those isometries s , such that

$$s : x \mapsto x, \quad s : C_x(\rho) \longrightarrow C_x(\rho).$$

Let us denote by $M_x(\rho)$ the order of the group $S_x(\rho)$. Since the rank of $C_x(2R)$ in a Delone set $X \subset \mathbb{R}^d$ equals d , the order $1 \leq M_x(\rho) < \infty$, i.e. the function $M_x(\rho)$ is defined for all $\rho \geq 2R$.

The function $M_x(\rho)$ for all $\rho \geq 2R$ takes positive integer values, is continuous on the left and non-increasing. Moreover, the ratio $M_x(\rho) : M_x(\rho')$ is integer if $\rho' > \rho$. In fact, it is obvious that the group $S_x(\rho')$ of a bigger cluster $C_x(\rho')$ either coincides with $S_x(\rho)$, or it is a proper subgroup of $S_x(\rho)$, $\rho' > \rho$.

Let X be a Delone set of finite type. Then for any positive ρ the set X splits into a finite number $N(\rho)$ of subsets $X_1, X_2, \dots, X_{N(\rho)}$, such that points x and x' from every one subset X_i have equivalent ρ -clusters $C_x(\rho)$ и $C_{x'}(\rho)$, but at points from different subsets X_i and X_j the ρ -clusters are not equivalent. The groups of equivalent ρ -clusters are conjugate in $Iso(d)$ and consequently have the same order $M_i(\rho)$, where i is the index of a subset X_i , $i \in [1, N(\rho)]$.

One of main goals of the local theory of regular systems is to determine a radius $\hat{\rho}$ such that any Delone set X (with parameters r and R) with $N(\hat{\rho}) = 1$ is a regular system. Certainly, the answer may depend on the dimension. So, for $d = 1$ it is easy to see that a Delone set on a line is a regular system if $N(2R) = 1$. The value $2R$ cannot be improved: in fact, for any $\varepsilon > 0$ there are Delone sets with $N(2R - \varepsilon) = 1$ that are not regular systems. The first important result in the local theory of regular systems was obtained in [5].

Theorem 2.1 (Local criterion for regular systems). *A Delone set $X \subset \mathbb{R}^d$ (with parameters r and R) is a regular system if and only if for some $\rho_0 > 0$ the following conditions hold:*

- (I) $N(\rho_0 + 2R) = 1$;
- (II) $M(\rho_0) = M(\rho_0 + 2R)$.

Condition (I) means that $(\rho_0 + 2R)$ -clusters at all points $x \in X$ are equivalent. Therefore the groups $S_x(\rho_0 + 2R)$ of the clusters are pairwise conjugate. Due to condition (II) for each point $x \in X$ the groups $S_x(\rho_0)$ and $S_x(\rho_0 + 2R)$ coincide.

Let us select among Delone sets with $N(2R) = 1$ *locally asymmetric* sets, i.e. such that the group $S_x(2R)$ is trivial. From the local criterion follows a theorem for locally asymmetric Delone sets.

Theorem 2.2 [Locally asymmetric sets]. *Let a Delone set $X \subset \mathbb{R}^d$ be locally asymmetric set and $N(4R) = 1$. Then X is a regular system, i.e. $N(\rho) \equiv 1, \forall \rho > 2R$.*

The theorem immediately follows from the criterion for $\rho_0 = 2R$.

It is amazing that due to the following theorem the condition $N(4R) = 1$ can not be reduced.

Theorem 2.3 ($(4R - \varepsilon)$ -theorem). *For any given $\varepsilon > 0$ and any dimension d , $d \geq 2$ there is a Delone set $X \subset \mathbb{R}^d$ such that $N(4R - \varepsilon) = 1$, but X is not a regular system.*

The theorem is proved by means of an explicit construction. Below we present such a design for dimension $d = 2$. This construction can be easily extended to any dimension d .

We start constructing the design with a rectangular lattice Λ (Fig. 2, on the left). The lattice Λ has a fundamental rectangle with side length a and b where $a \ll b$. It is clear that the parameter $R = \sqrt{b^2 + a^2}/2$. Since $a \ll b$ we have

$$2R \sim b(1 + a/2b) = b + a/2.$$

Horizontal rows of the Λ form a bi-infinite sequence with indices $i \in \mathbb{Z}$. The set of the rows splits into couples P_{2i} of rows with sequel indices $(i, i + 1)$ where the first

$$\dots RRR \dots \quad \dots RLRL \dots \quad \dots RLL \dots$$

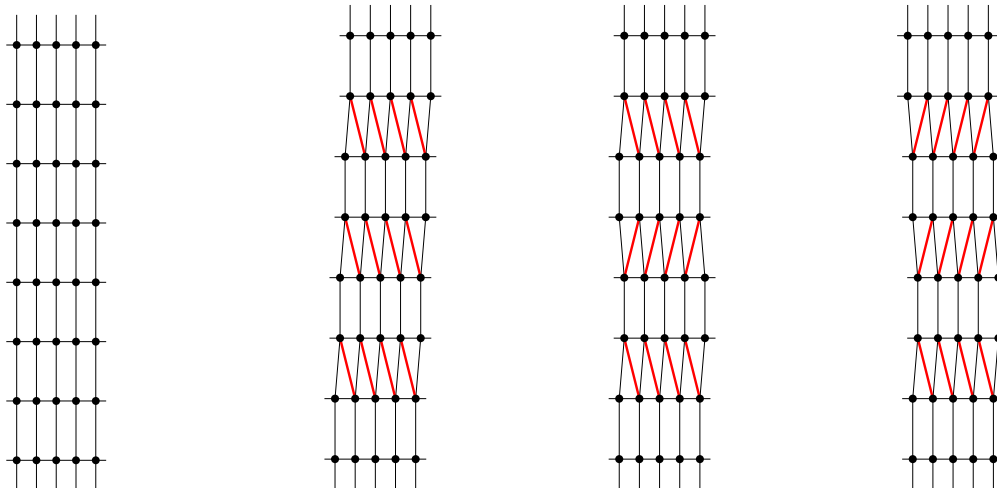


Fig.2

one i is even. Let us take c so that $0 < c < a/2$ and shift **each** couple P_{i+1} relatively to the previous couple P_i by c to the left or to the right.

We get a sequence of mutually shifted rows that can be encoded a bi-infinite sequence $l = \dots RLLRL \dots$. There are uncountably many different bi-infinite binary sequences $\{l\}$. The corresponding Delone sets X_l have the same parameters r and R . Among the sequences $\{l\}$ there are exactly 3 ones such that the corresponding Delone sets are regular systems. Two sequences $\dots LLLL \dots$ and $\dots RRRR \dots$ generate two congruent each other regular systems. The third bi-infinite sequence $\dots RLRLRL \dots$ encodes one more regular system to be mirror symmetrical to itself. All the other Delone sets from the family are not regular systems, though as it is easy to see that all of them have the same b -clusters $C_x(b)$. Since $b \sim 2R - a/2$ and $a > 0$ can be chosen arbitrarily small, we get the theorem.

In this context it is particularly interesting to note that there are the following results for Delone sets in an Euclidean plane and in 3D space:

Theorem 2.5 (Regular systems, $d = 2, 3$).

- (1) Let $X \subset \mathbb{R}^2$ be a Delone set in plane, if $N(4R) = 1$, then X is a regular system.
- (2) Let and $X \subset \mathbb{R}^3$ be a Delone set, if $N(10R) = 1$, then X is a regular system.

This result was obtained by M. Stogrin and by N. Dolbilin independently years ago; however a (complete) proof remains unpublished if one does not take into account publications on key ideas. As for point (1) of theorem 2.5, case $d = 2$, here we just mention that the part of the theorem can be derived from the following theorem:

Theorem 2.6 [15]. A tiling of Euclidean plane by convex polygons is regular, i.e. a tiling with a transitive symmetry group, if all first coronas are equivalent.

Details of the proof of the $10R$ -theorem for regular systems in \mathbb{R}^3 will appear in [14]. Here we just mention that, due to the $(4R - \varepsilon)$ -theorem, the estimate $4R$ for plane is the best estimate. As for the estimate $10R$ for 3D-space, it looks much higher than the actual one. The difficulty lies in the fact that we can not deal effectively with the $4R$ -cluster group.

In this regard, it is especially remarkable that in the case where the $2R$ -cluster group contains the central symmetry, a sufficient condition on regular systems becomes extremely simple and holds for any dimension.

Definition 2.6. A Delone set X is called a *locally antipodal* set if the $2R$ -cluster $C_x(2R)$ for each point $x \in X$ is centrally symmetrical about the cluster center x .

Now we present several theorems to be proved in the next sections.

Theorem 1 . *If X is a locally antipodal set and $N(2R) = 1$, then X is a regular system.*

Theorem 2. *A locally antipodal Delone set X is centrally symmetrical about each point $x \in X$ globally.*

We emphasize that in either theorem 2 or in the following theorem 3, no condition on the cluster counting function $N(\rho)$ is required. Moreover, we do not require even that a Delone set X is of finite type.

Theorem 3. *A locally antipodal Delone set $X \subset \mathbb{R}^d$ is a crystal. Moreover, X is the disjoint union of at most $2^d - 1$ congruent and parallel lattices:*

$$X = \bigsqcup_{i=1}^n (x + \lambda_i/2 + \Lambda),$$

where Λ is the maximum lattice for X such that $X + \Lambda = X$, $\lambda_i \in \Lambda$ and $\lambda_i \equiv \lambda_j \pmod{2} \Leftrightarrow i = j$, $n < 2^d$.

Theorems 1– 3 have been published in part in [7] and [8]. In this paper theorems 1 and 2 are easily derived from the following theorem.

Theorem 4 (Uniqueness theorem). *Let X and Y be Delone sets with the parameter R , suppose they have a point x in common. Let the $2R$ -clusters of X and Y centered at this point x coincide, i.e. $C_x(2R) = C'_x(2R)$, where $C_x(\rho)$ stands for a cluster in X and $C'_y(\rho)$ for a cluster in Y . Then $X = Y$.*

In the conclusion to this section we present a local criterion for a crystal. This criterion generalizes the local criterion for regular systems. It was announced [6] and proved a while ago but a full proof was published recently [7] (in Russian). The proof in this paper is a slight improvement of the proof in [7].

Theorem 5 (Local criterion for a crystal). *A Delone set X of finite type is a crystal which consists of m regular systems if and only if there is some $\rho_0 > 0$ such that two conditions hold:*

- 1) $N(\rho_0) = N(\rho_0 + 2R) = m$;
- 2) $S_x(\rho_0) = S_x(\rho_0 + 2R), \forall x \in X$.

The local criterion for regular systems (theorem 2.1) is a particular case of theorem 5. Indeed, the condition $N(\rho_0 + 2R) = 1$ implies $N(\rho_0) = N(\rho_0 + 2R) = 1$. The cluster groups $S_x(\rho)$ for all $x \in X$ are pairwise conjugate, hence it suffices to require $S_x(\rho_0) = S_x(\rho_0 + 2R)$ for one point from X only.

3 Proof of the Local Criterion for a Crystal

First of all we make some comments on conditions 1) and 2) of theorem 5. Condition 1) means that with increasing radius ρ the number of cluster classes on segment $[\rho_0, \rho_0 + 2R]$ does not increase, i.e. remains unchanged: $N(\rho) = N(\rho + 2R)$.

In addition, due to condition 2), the cluster group $S_x(\rho_0)$, $\forall x \in X$, does not get smaller under the $2R$ -extension of ρ_0 -cluster: $S_x(\rho_0) = S_x(\rho_0 + 2R)$. The key point of theorem 5 is that the stabilization of these two parameters (the number of cluster classes and the order of cluster groups) on segment $[\rho_0, \rho_0 + 2R]$ implies their stabilization on the rest of the half-line $[\rho_0 + 2R, \infty)$.

Лемма 3.1 (on the $2R$ -chain). *For any pair of points x and $x' \in X$, where X is a Delone set, in X there is a finite sequence $x_1 = x, x_2, \dots, x_k = x'$, such that $|x_i x_{i+1}| < 2R$ $\forall i \in [1, k-1]$.*

We omit a proof of the lemma which can be found in, e.g. [5].

We recall that X splits into disjoint subsets $X = \bigsqcup_{i=1}^m X_i$, where X_i is a subset of all points of X whose ρ_0 -clusters are pairwise equivalent and belong to the i -th class.

Лемма 3.2 (on the $2R$ -extension). *Let a Delone set X fulfil conditions 1) and 2) of theorem 5 and $x, x' \in X_i$. Let $f \in \text{Iso}(d)$ be an isometry such that*

$$f : x \mapsto x' \text{ and } f : C_x(\rho_0) \rightarrow C_{x'}(\rho_0). \quad (1)$$

Then the same isometry f superposes the concentrically bigger cluster $C_x(\rho_0 + 2R)$ onto cluster $C_{x'}(\rho_0 + 2R)$:

$$f : C_x(\rho_0 + 2R) \rightarrow C_{x'}(\rho_0 + 2R). \quad (2)$$

Proof. If the ρ -clusters $C_x(\rho)$ and $C_{x'}(\rho)$ are equivalent, by condition 1) of theorem 5, the corresponding $(\rho_0 + 2R)$ -clusters are equivalent too. Therefore there is an isometry g such that

$$g : C_x(\rho_0 + 2R) \rightarrow C_{x'}(\rho_0 + 2R).$$

If $g = f$ the lemma is already proved. Now we assume $f \neq g$ we consider the superposition of isometries $f^{-1} \circ g$. The order here is from the right to the left: g is applied first, followed by f^{-1} .

$$f^{-1}(g(C_x(\rho_0))) = f^{-1}(C_{x'}(\rho_0)) = C_x(\rho_0).$$

We have:

$$f^{-1} \circ g : x \mapsto x \text{ and } f^{-1} \circ g : C_x(\rho_0) \rightarrow C_x(\rho_0). \quad (3)$$

Relationship (3) shows that $f^{-1} \circ g$ is a symmetry s of the ρ -cluster $C_x(\rho_0)$: $s \in S_x(\rho_0)$. By condition 2) of theorem 5 we also have $s \in S_x(\rho_0 + 2R)$. The relation $f^{-1} \circ g = s$ implies $g \circ s^{-1} = f$. Therefore one gets

$$\begin{aligned} f(C_x(\rho_0 + 2R)) &= (g \circ s^{-1})(C_x(\rho_0 + 2R)) = \\ &= g(s^{-1}(C_x(\rho_0 + 2R))) = g(C_x(\rho_0 + 2R)) = C_{x'}(\rho_0 + 2R). \end{aligned}$$

□

Лемма 3.3 (Main Lemma). . Let a Delone set X fulfil conditions 1) and 2) of theorem 5 and X_i a subset of X of all points whose ρ_0 -clusters belong to the i -th class, $i \in [1, m]$. Let a group $G_i = \langle f \rangle$ be generated by all isometries f such that $f : C_x(\rho_0) \rightarrow C_{x'}(\rho_0)$, $\forall x, x' \in X_i$. Then G_i operates transitively on every set X_j , $\forall j \in [1, m]$. Moreover, the group G_i does not depend on i , $G_i = \text{Sym}(X)$.

Proof. In fact, since for x and $x' \in X_i$ the ρ_0 -clusters $C_x(\rho_0)$ and $C_{x'}(\rho_0)$ are equivalent, there are several isometries superposing these clusters. The number of these isometries is equal to the order $|S_x(\rho_0)|$ of the cluster group.

We prove that if f is one of these isometries, then f is a symmetry of the whole X . First we take an arbitrary point $y \in X$ and prove that its image $f(y)$ belongs to X (see Fig.3). Let us connect points x and y with a $2R$ -chain \mathcal{L} :

$$\mathcal{L} = \{x_1 = x, x_2, \dots, x_n = y : |x_i x_{i+1}| < 2R, \forall i \in [1, n-1]\}.$$

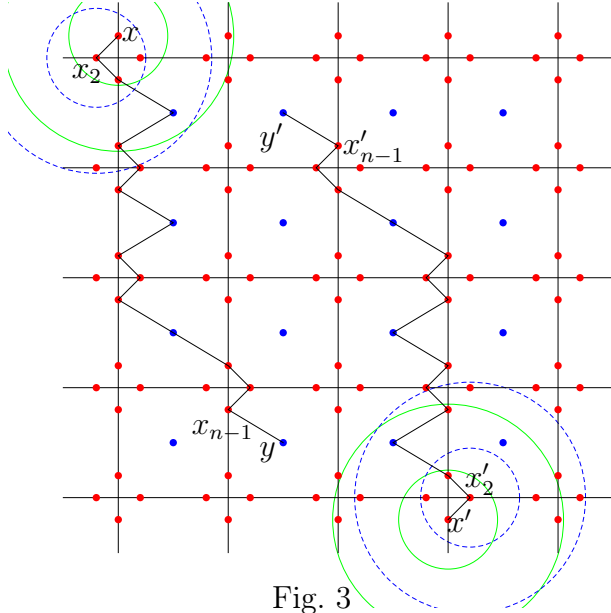


Fig. 3

Since $f(C_{x_1}(\rho_0)) = C_{x'_1}(\rho_0)$, then by Lemma 3.2

$$f(C_{x_1}(\rho_0 + 2R)) = C_{x'_1}(\rho_0 + 2R). \quad (4)$$

Since $|x_1 x_2| < 2R$ we have

$$C_{x_2}(\rho_0) \subset C_{x_1}(\rho_0 + 2R).$$

Therefore relation (4) implies:

$$f : C_{x_2}(\rho_0) \rightarrow C_{x'_2}(\rho_0).$$

By lemma 3.2 we have

$$f : C_{x_2}(\rho_0 + 2R) \rightarrow C_{x'_2}(\rho_0 + 2R). \quad (5)$$

From the inequality $|x_2 x_3| < 2R$ it follows that

$$C_{x_3}(\rho_0) \subset C_{x_2}(\rho_0 + 2R).$$

Therefore due to (5) we have:

$$f : C_{x_3}(\rho_0) \rightarrow C_{x'_3}(\rho_0).$$

By Lemma 3.2 we have again:

$$f : C_{x_3}(\rho_0 + 2R) \rightarrow C_{x'_3}(\rho_0 + 2R).$$

Moving along chain \mathcal{L} and repeating this argument finitely many times we get that the $2R$ -chain $\mathcal{L} \subset X$ is moved by isometry f into a $2R$ -chain $\mathcal{L}' \subset X$. The endpoint y of the first chain \mathcal{L} moves into the endpoint y' of the second one. Thus, it is shown that the isometry f maps X **into** X : $f(X) \subseteq X$.

We show now that this map is a map **onto** the whole X : $f(X) \supseteq X$. Let us take an arbitrary point $y'' \in X$ and show that its pre-image $f^{-1}(y'')$ also belongs to X . For the inverse mapping f^{-1} from relation (4) it follows:

$$f^{-1} : C_{x'_1}(\rho_0 + 2R) \rightarrow C_{x_1}(\rho_0 + 2R).$$

Let us again connect points x'_1 and y'' with a $2R$ -chain. Moving along the chain by means of the same argument we get $f^{-1}(y'') = x'' \in X$. Finally, the mapping f moves some point x'' into the a priori chosen point y'' : $f(x'') = y''$.

Now we take a group $G_i = \langle f \rangle$, where f are all isometries of $Iso(d)$ which superpose the clusters $C_x(\rho_0)$ and $C_{x'}(\rho_0)$, $x, x' \in X_i$. We have proved that G_i belongs to the group $G := \text{Sym}(X)$ (i.e. $G_i \subseteq G$) and the group G_i operates on X_i transitively. In order to complete the proof of Lemma 3.3 one needs to show that $G_i \supseteq G$ for each $i \in [1, m]$. Indeed, we show that if $g \in G$, then $g \in G_i$. It is the case because g is a symmetry of X and, hence, moves any point $y \in X_i$ and its ρ_0 -cluster $C_y(\rho_0)$ into a point $g(y) \in X_i$ and the cluster $C_{g(y)}(\rho_0)$, respectively. By the above-proved, the symmetry g belongs to the group G_i , i.e. $G_i \supseteq G$. So, we proved that $G_i = \text{Sym}(X)$. \square

So, we have proved that a Delone set X with conditions 1) and 2) of Theorem 5 is partitioned into the union of m disjoint discrete sets X_i such that each subset X_i is a $\text{Sym}(X)$ -orbit of some point. In order to prove Theorem 5 we need to make sure that $\text{Sym}(X)$ is a crystallographic group. A proof of this fact is divided into two lemmas:

Лемма 3.4. *Assume that a group $G \subset Iso(d)$ is such that for some point $x \in \mathbb{R}^d$ its orbit $G \cdot x$ is a Delone set, then G is a crystallographic group.*

Лемма 3.5. *In a partition $X = \bigsqcup_i^m X_i$ each subset X_i is a Delone set.*

From these two lemmas it follows that X is a crystallographic orbit of finite set of m points, i.e. that X is a crystal with respect to the group G . In fact, let us take a Delone subset X_i , which exists by lemma 3.5, and a group $G = G_i = \text{Sym}(X)$ generated by all possible isometries f as in Lemma 3.3. Since $G \cdot x = X_i$ where $x \in X_i$, by Lemma 2.4 the group G is crystallographic. Let a finite point set X_0 consist of m representatives of subsets X_i , $i \in [1, m]$. Then $X = G \cdot X_0$. We get that that X is a

crystallographic orbit of the finite set X_0 , i.e. X is a crystal. This completes the proof of the local criterion.

Now we prove the last two lemmas.

Proof of Lemma 3.4. Let $X := G \cdot x$, (in Lemma 3.4 G is not assumed necessarily to be the full symmetry group $\text{Sym}(X)$ of X , i.e. $G \subseteq \text{Sym}(X)$). Let \mathcal{V} denote the Voronoi tiling of space \mathbb{R}^d with respect to X . A Voronoi domain V_x for the point $x \in X$ is a cell of the tiling \mathcal{V} . V_x is a convex d -polytope with a finite number of facets. This number of facets can be easily estimated from above in terms of parameters r and R . Therefore the symmetry group $\text{Sym}(V_x)$ of V_x is also finite. Moreover, the order $|\text{Sym}(V_x)|$ of this group can be also bounded from above depending on the same parameters r and R .

Every symmetry of the Delone set X leaves the Voronoi tiling \mathcal{V} invariant. Therefore, since the group G operates on the X transitively, this group also operates transitively on the set of all cells of the tiling \mathcal{V} . It is obvious that the following inclusions are true: $G \subseteq \text{Sym}(X) \subseteq \text{Sym}(\mathcal{V})$.

The orbit $\text{Sym}(\mathcal{V}) \cdot y$ of any point $y \in \mathbb{R}^d$ is a discrete set because the orbit $\text{Sym}(\mathcal{V}) \cdot y$ and Voronoi polytope V_x intersect in a finite set:

$$|\text{Sym}(\mathcal{V}) \cdot y \cap V_x| \leq |\text{Sym}(V_x)| < c(r, R, d).$$

Therefore $\text{Sym}(X)$ is discrete. Since G is a subgroup of $\text{Sym}(X)$, it is also discrete.

As for the fundamental domain $F(G)$, it can be chosen as $V_x/\text{stab}(x)$ where $\text{stab}(x)$ is the stabilizer of the point x in G . In particular, if the stabilizer is trivial then the fundamental domain $F(G)$ is the Voronoi polytope V_x . Thus, the fundamental domain $F(G)$ is compact and hence G is a crystallographic group. \square

Proof of Lemma 3.5. First of all, we note that since X is a Delone set with parameter r , any subset X_i fulfils the (r) -condition of Delone set with a parameter r' , where $r' \geq r$.

We suppose that there is a subset X_i which does not satisfy the second condition of Delone set for any finite value R' . In this case there is an infinite sequence of balls $B_1, B_2, \dots, B_k, \dots$ empty of points of X_i with infinitely increasing radii: $R_1 < R_2 < \dots < R_k < \dots \rightarrow \infty$. Since the set X_i is discrete, each of these balls B_k can be moved so that on its boundary there is a point $x_k \in X_i$. Since all the points $x_k \in X_i$ belong to the G -orbit, one can move every point x_k along with the ball B_k to some given point $x \in X_i$ by means of an appropriate isometry $f_k \in G$. Thus, one can assume that the point x is on the boundary of an empty ball B'_k of radius R_k for every $k = 1, 2, \dots$. Let \mathbf{n}_k denote a unit vector

$$\mathbf{n}_k := \frac{1}{|xO_k|} \overrightarrow{xO_k},$$

where O_k is the center of ball B'_k . Now we select from sequence $\{\mathbf{n}_k\}$ a subsequence $\mathbf{n}_{k_j} \rightarrow \mathbf{n}$ that converges to a unit vector \mathbf{n} .

Let Π be a hyperplane through point x orthogonal to a vector \mathbf{n} , Π^+ the **open** half-space where the normal vector \mathbf{n} points in. The half-space Π^+ contains no points of X_1 . In fact, given a point $z \in \Pi^+$, in the subsequence of balls with infinitely increasing radii one can find a ball B_{k_j} which contains point z . Since all balls B_{k_j} are empty of points of X_i , $z \notin X_i$.

Thus, all points of X_i are in a **closed** half-space Π^- . We admit that all the points of X_i can lay on the hyperplane Π itself. Since X is a Delone set, the open half-space Π^+ also contains points of X .

Given $i \in [1, m]$ and $x \in X_i$, we take $\mathfrak{x} \neq i$ and choose in X_j a point y closest to $x \in X_i$. One should note that since X_j is a discrete set, such a point y does exist. Generally, there can be several but always finitely many closest points. Let us denote $\delta(x, X_j) := \min_{y \in Y_j} |xy|$. Since G operates transitively on both sets X_i and X_j , the minimum $\delta(x, X_j)$ does not depend on the choice of point $x \in Y_i$, i.e. for any other point $x' \in X_i$ there is a point $y' \in X_j$ with condition $\delta(x', X_j) := \delta_{ij}$. It is clear also that $\delta_{ij} = \delta_{ji}$. Now one can denote

$$\delta_i := \max_{j \in [1, m], j \neq i} \delta_{ij}.$$

It is clear that for every $j \in [1, m]$, $j \neq i$, and $\forall y \in X_j$ there is a point x of X_i at distance from y of no bigger than δ_i .

Therefore, since the subset X_i is supposed to be located in the closed half-space Π^- the whole set X is located in a half-space $(\Pi + \delta_i \mathbf{n})^-$ determined by hyperplane $\Pi + \delta_i \mathbf{n}$. The obtained contradiction to the R -condition of the Delone set X completes a proof of Lemma 3.5. \square

4 Proof of Theorem 4

At first we will prove Theorem 4. This theorem easily implies Theorems 1 and 2. The proof of Theorem 3 is based, in part on Theorem 2. We note that in Theorem 4 the locally antipodal Delone sets X and Y a priori are not required to be sets of finite type.

Let us take an arbitrary point $x \in X$ and define the *distance spectrum* at the x as the taken in ascending order set of distances between the point x and the other points of X :

$$\mathfrak{R}_x := \{\rho \in R_+ | \exists x' \in X, |xx'| = \rho\}.$$

By the r -condition for X the spectrum \mathfrak{R}_x is discrete and has no limit points (with the exception of ∞) for any given $x \in X$. Now we consider the union $\cup_{x \in X} \mathfrak{R}_x$ over all $x \in X$. It is easy to see that the union $\cup_{x \in X} \mathfrak{R}_x$ of the spectra over all points of X is a discrete set with no proper limit point if and only if the Delone set X is of finite type.

Recall conditions for Delone sets X and Y : $x \in X \cap Y$ and $C_x(2R) = C'_x(2R)$. $C'_y(\rho)$ stands for the ρ -cluster in the set Y). We take the point x and the two distance spectra $\mathfrak{R}_x = \{\rho_1 < \rho_2 < \dots\}$ and $\mathfrak{R}'_x = \{\rho'_1, \rho'_2, \dots\}$ in X and in Y , respectively, and prove the total coincidence of the spectra \mathfrak{R}_x and \mathfrak{R}'_x and the sets X and Y by induction along numbers k of distance sequences ρ_k and ρ'_k .

Due to the condition $C_x(2R) = C'_x(2R)$, some initial portions of the spectra \mathfrak{R}_x and \mathfrak{R}'_x coincide. Assume that we have already proved the equality of the first k distances $\rho_1 = \rho'_1, \dots, \rho_k = \rho'_k$ in the spectra and the coincidence of the clusters $C_x(\rho_k) = C'_x(\rho_k)$.

Now we prove that $\rho_{k+1} = \rho'_{k+1}$ and $C_x(\rho_{k+1}) = C'_x(\rho'_{k+1})$. Let $\rho_{k+1} \leq \rho'_{k+1}$, then the ball $B_x(\rho_{k+1})$ has on its boundary at least one point $x_1 \in X$, $|xx_1| = \rho_{k+1}$ (see Fig. 4). Let $z \in \mathbb{R}^d$ be such that $z \in [xx_1]$ and the length $|zx_1| = R$. We note that point z , generally, does not belong to X . The ball $B_z(R)$ centered at z of radius R touches the sphere $\partial B_x(\rho_{k+1})$ at point x_1 . Now let h be the homothety with the center

x_1 and the coefficient 2 and $B_{z'}(2R) := h(B_z(R))$ (see Fig. 4). It is obvious that we have

$$B_z(R) \subset B_{z'}(2R) \subset B_x^o(\rho_{k+1}) \cup \{x_1\}. \quad (2)$$

Here B^o means an open ball.

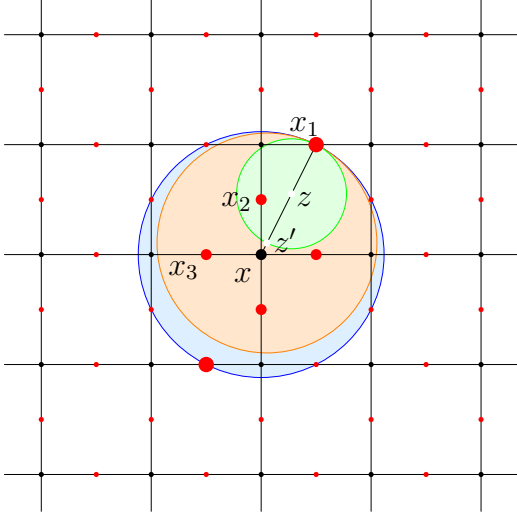


Fig. 4

By the R -condition, in $B_z(R)$ there is at least one point $x_2 \in X$, $x_2 \neq x_1$. Since x_1 is the only point of the ball $B_z(R)$ which is located on the boundary $\partial B_x(\rho_{k+1})$, all other points of $B_z(R)$, including the point x_2 , lay in the interior of $B_x(\rho_{k+1})$. Therefore $|xx_2| < |xx_1| = \rho_{k+1}$, i.e. $|xx_2| \leq \rho_k$, and, by the induction assumption, $x_2 \in X \cap Y$. Since $|x_1x_2| \leq 2R$ the point x_1 belongs to the cluster $C_{x_2}(2R)$.

Since the cluster $C_{x_2}(2R)$ is antipodal about x_2 , in this cluster there is a point x_3 which is antipodal to x_1 . We recall that the coefficient of the homothety h equals 2, hence

$$x_3 \in B_{z'}(2R) \subset B_x^o(\rho_{k+1}) \cup \{x_1\}.$$

Therefore, $|xx_3| \leq \rho_k$, as well as $|xx_2| \leq \rho_k$, and, by the inductive assumption, $x_2, x_3 \in Y$. Since $|x_2x_3| \leq 2R$, we have that $x_3 \in C'_{x_2}(2R)$. Now, since x_1 is antipodal to x_3 about x_2 and the cluster $C'_{x_2}(2R)$ is antipodal about x_2 , x_1 also belongs to $C'_{x_2}(2R)$. Hence we have also $x_1 \in Y$. This inclusion is true for any $x'_1 \in X$ with $|xx'_1| = \rho_{k+1}$. Thus, it has been proved that if $\rho_{k+1} \leq \rho'_{k+1}$ we actually have $\rho_{k+1} = \rho'_{k+1}$. Therefore we just proved $C_x(\rho_{k+1}) \subseteq C'_x(\rho_{k+1})$. However, in the case $\rho_{k+1} = \rho'_{k+1}$ one can also take any point $y_1 \in Y$ with $|xy_1| = \rho_{k+1}$ and by the same argument prove that $y_1 \in X$. Thus, the inductive step is established: one has proved that $C_x(\rho_{k+1}) = C'_x(\rho_{k+1})$. \square

5 Proofs of Theorems 1,2, and 3

Theorems 1 and 2 easily follow from Theorem 4.

Proof of Theorem 1. By the requirement $N(2R) = 1$, for any x' and $x \in X$ there is an isometry g such that $g(x') = x$ and $g(C_{x'}(2R)) = C_x(2R)$. Let us denote $Y := g(X)$. We have two local antipodal sets X and Y such that $X \cap Y \supseteq C_x(2R)$. By Theorem 4, the relationship $C_x(2R) = C_{x'}(2R)$ implies $X = Y$, i.e. g is a symmetry of X . Thus $\text{Sym}(X)$ possesses transitive symmetry group. \square

Proof of Theorem 2. X is a locally antipodal Delone set. Let σ_x be the inversion about a point x such that $\sigma_x : C_x(2R) \rightarrow C_x(2R)$. Let us denote $Y := \sigma(X)$. Then we have again two sets X and Y with a $2R$ -cluster $C_x(2R)$ in common. By Theorem 4 we have $X = Y$, i.e. the inversion σ_x leaves the set X invariant. \square

Proof of Theorem 3

Given a locally antipodal set $X \subset \mathbb{R}^d$, let Λ be a set of vectors λ such that $X + \Lambda = X$. Since X is discrete the vector set Λ is a lattice.

Now we show that the lattice Λ is a lattice of rank d . Indeed, let σ_x and $\sigma_{x'}$ be inversions of clusters $C_x(2R)$ and $C_{x'}(2R)$ at points x and x' , respectively. Then, by Theorem 2, they are both symmetries of the whole X . On the other hand, the superposition $\sigma_x \circ \sigma_{x'}$ is a translation by the vector $2(x - x')$. Since the set X is a Delone set, the translational group Λ generated by all possible $2(x - x')$, where $x, x' \in X$, is a lattice of the rank d . Λ is the maximum lattice to leave X invariant, i.e. such that $X + \Lambda = X$.

The Delone set X is the union of finitely many lattices which are congruent and parallel to the lattice Λ , i.e.

$$X = \bigcup_{i=1}^n (x_i + \Lambda).$$

As proved above, for $i = 2, 3, \dots, n$ we have $x_i - x_1 \in \Lambda/2$.

By putting $x := x_1$, $\lambda_i/2 = x_i - x_1$ ($i = 1, 2, \dots, n$) we come to:

$$X = \bigsqcup_{i=1}^n (x + \lambda_i/2 + \Lambda), \text{ where } \lambda_i \in \Lambda. \quad (6)$$

Now, if $\lambda_i \equiv \lambda_j \pmod{2}$, i.e. if $\lambda_i - \lambda_j = 2\lambda$, where $\lambda \in \Lambda$, then subsets $x + \lambda_i + \Lambda$ and $x + \lambda_j + \Lambda$ obviously coincide. Therefore in (6) $n \leq 2^d$. Moreover, the value n cannot be equal to 2^d because in this case $X = \Lambda/2$ and hence $X + \Lambda/2 = X$. This contradicts the assumption that Λ is the maximum lattice with the condition $X + \Lambda$. So, $n \leq 2^d - 1$. \square

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